WHAT IS CLAIMED IS:

1. A method of identifying a three-dimensional molecular structure, comprising:

accessing a computer readable representation of a reference structure having a plurality of residues;

calculating interaction between said plurality of residues and the molecular structure; and

producing a residue fingerprint based on said interaction to identify the molecular structure.

2. The method according to claim 1, wherein said calculating step comprises:

computing inter-atomic distance between the molecular structure and a residue from said plurality of residues; and

denoting said residue as an interacting residue when the inter-atomic distance is less than a predetermined threshold.

3. The method according to claim 2, wherein said producing step comprises:

identifying said interacting residue in said residue fingerprint.

4. The method according to claim 2, further comprising:

deriving said predetermined threshold from the van der Waals radius of an atom from the molecular structure.

5. The method according to claim 2, wherein said computing step comprises:

computing inter-atomic distance between at least one atom of the molecular structure and at least one atom of said residue.

6. The method according to claim 1, wherein said producing step comprises:

generating a binary representation of a listing of interacting residues from said plurality of residues to, thereby, produce said residue fingerprint, each interacting residue having an inter-atomic distance from the molecular structure less than a predetermined threshold.

7. The method according to claim 1, further comprising:

comparing each type of atom in the molecular structure with each type of atom in a residue from said plurality of residues to detect an interacting residue having an inter-atomic distance below a predetermined threshold.

8. The method according to claim 1, further comprising:

comparing the molecular structure with each type of atom in a residue from said plurality of residues to detect an interacting residue having an inter-atomic distance below a predetermined threshold.

9. The method according to claim 1, further comprising:

comparing the molecular structure with each type of atom in a residue from said plurality of residues to detect an interacting residue having an inter-atomic distance below a predetermined threshold;

computing the number of each type of interaction; and

including, in said residue fingerprint, a listing of interacting residues and an associated number of each type of interaction.

10. The method according to claim 1, further comprising:

comparing the molecular structure with each type of atom in a residue from said plurality of residues to detect an interacting residue having an inter-atomic distance below a predetermined threshold;

distinguishing the specific atoms on said interacting residue; and

including, in said residue fingerprint, a listing of interacting residues and the associated specific atoms for each interacting residue.

11. The method according to claim 1, further comprising:

calculating interaction between said plurality of residues and a second molecular structure to produce a second residue fingerprint; and

computing the similarity between the molecular structure and said second molecular structure based on said residue fingerprint and said second residue fingerprint.

12. A method of identifying a plurality of three-dimensional molecular structures, comprising:

accessing a reference structure having a plurality of residues;

calculating interaction between said plurality of residues and each of the plurality of molecular structures; and

producing a plurality of residue fingerprints based on said interaction, each residue fingerprint characterizing a corresponding molecular structure from the plurality of molecular structures.

13. The method according to claim 12, further comprising:

classifying the plurality of molecular structures into clusters based on said plurality of residue fingerprints, each cluster of molecular structures having a similar binding mode.

14. The method according to claim 13, further comprising:

computing a Tanimoto score among the molecular structures in each cluster of the plurality of molecular structures, wherein each pair of structures within a cluster of molecular structures has a similar Tanimoto score.

15. A computer program product comprising a computer useable medium having computer readable program code functions embedded in said medium for causing a computer to identify a three-dimensional molecular structure, comprising:

a first computer readable program code function that causes the computer to access a reference structure having a plurality of residues;

a second computer readable program code function that causes the computer to calculate interaction between said plurality of residues and the molecular structure; and

a third computer readable program code function that causes the computer to produce a residue fingerprint based on said interaction to identify the molecular structure.

16. The computer program product according to claim 15, wherein said second computer readable program code function comprises:

a fourth computer readable program code function that causes the computer to detect an interacting residue having a distance between the molecular structure and said residue below a predetermined threshold, wherein said residue fingerprint includes a listing of interacting residues.

17. The computer program product according to claim 15, further comprising:

a fourth computer readable program code function that causes the computer to create a binary representation of a listing of interacting residues from said plurality of residues to, thereby, produce said residue

fingerprint, wherein each interacting residue has an inter-atomic distance from the molecular structure less than a predetermined threshold.